

## **PhD Position in Designing CO<sub>2</sub> Photocapture Materials and performing their Life-cycle and Technoeconomic Assessments**

This position is funded through a collaborative project between Prof. Kulbir Ghuman at the Institut National de la Recherche Scientifique (INRS) and Prof. Paul O'Brien at the Lassonde School of Engineering, York University

### **Project title: Nano- to Gigascale Development and Modelling of CO<sub>2</sub> Photocapture Materials**

**Project description:** The successful applicant will work on an exciting research project that has the potential to push sustainable energy technologies beyond their current limits. The high level research objectives of this project are to (1) model materials that exhibit selective CO<sub>2</sub> photoadsorption at the nanoscale and (2) perform technoeconomic (TEA) and life-cycle assessment (LCA) for systems that use these materials to capture CO<sub>2</sub> at a globally significant rates. Density Functional Theory (DFT) and Time-Dependent DFT (TDDFT) will be used to understand CO<sub>2</sub> adsorption photoactivity. The cost-effectiveness of CO<sub>2</sub> capture systems will be estimated using TEA and the environmental impacts of the CO<sub>2</sub> capture systems will be predicted by following the ISO 14044 guidelines for LCA. By aligning the goals, scope and other parameters of LCA and TEA, both financial and environmental aspects of a technology can be evaluated. This analysis will be performed for multiple operating scenarios (i.e. different locations, energy sources, and applications or end uses for the captured CO<sub>2</sub>).

**Research area:** Sustainable energy, Computational materials design, Nanomaterials, Life cycle assessment, Technoeconomic analysis

**Research advisors:** Prof. Kulbir Ghuman, Prof. Paul O'Brien

**Starting date:** Jan 2021 or May 2021

**Institution:** Lassonde School of Engineering, York University, 4700 Keele St., Toronto, Ontario, M3J 1P3, Canada & Institut National de la Recherche Scientifique, Centre Énergie Matériaux Télécommunications, 1650 Boulevard Lionel-Boulet, Varennes, Quebec, J3X 1S2, Canada

**Financial support:** All students are entitled to receive financial support during their graduate studies. Moreover, students are also invited to apply for external scholarships from FRQNT, NSERC, etc.

**Eligibility:** Applicants should have a degree (M.Sc. or M.A.Sc) in Engineering, Materials Science, Physics, Chemistry, or equivalent and must be fluent in English (orally as well as in written). Fluency in French is considered to be a valuable asset. He/She should be able to work independently as well as with a team. His/Her ability to demonstrate critical and independent thinking will be invaluable assets.

**How to apply:** Interested candidates should send a detailed CV, cover letter, academic records, statement of interest, and the contact details of at least one reference to [paul.obrien@lassonde.yorku.ca](mailto:paul.obrien@lassonde.yorku.ca) or [kulbir.ghuman@emt.inrs.ca](mailto:kulbir.ghuman@emt.inrs.ca). Please mention if you are an international or a domestic (Canadian citizen/permanent resident) candidate. Any inquiries can also be sent to these emails.